Path-integral approach of ionization by ultrashort laser pulses

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In the present paper, we model in a fully quantum-mechanical way the dynamics of an atom with one active electron interacting with a coherent linearly polarized ultrashort photonic pulse. We use path-integral methods. We derive the system's propagator in its discrete form and develop a Monte Carlo method to study its dynamics. To avoid any additional complication, we apply our method to the ionization of atomic hydrogen from its ground state supposing that the photon energy is greater than the ionization threshold and give the ionization probability. In fact, the present method can be applied to the ionization of any atom or molecule.

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I. INTRODUCTION

The study of the interaction of atoms with radiation is an interesting and long-standing area of research in classical, semiclassical, and quantum physics [1–3]. The development of lasers opened new horizons in that study. In the past two decades there have appeared numerous investigations in the study of laser atom interaction both in theory and in experiment (see, for example, [4–8]) and interesting mechanisms, such as the dynamical stabilization [9].

A further boost was given by the achievement in laboratories of ultraviolet laser pulses in the femtosecond and further in the attosecond regime [10,11]. Such pulses have the possibility to ionize an atom via a single photon. Additionally, due to their short duration the ionization takes place in a time interval shorter than any relaxation period of the system under consideration. Many methods have been introduced in order for such systems to be studied [12,13]. Moreover, such pulses can be captured in cavities by using certain experimental configurations [14].

In the present paper, we introduce a fully quantum-mechanical field-theoretical treatment for the interaction of an atom with an ultrashort coherent pulse, as a rigorous alternative to methods such as the direct solution of the time-dependent Schrödinger equation. As an application, we consider the photoionization of H by a coherent pulse in the subfemtosecond regime. We treat the problem via path-integral methods. We calculate the photoionization probability versus time for various pulse durations. We restrict ourselves to the weak-field limit as otherwise a system with a strong field can be treated in a semiclassical way. The solution of the problem follows with similar steps to those in Refs. [15–18], i.e., we first integrate the field variables using the coherent-state path-integral formalism and then we integrate the path integral over the electron space variables. In fact, by using a Monte Carlo method our method circumvents the complete solution of the time-dependent Schrödinger equation. Since we use a weak field, we are able to keep only the photonic field-free terms in a possible perturbation expansion of the initial and the final state with respect to the photonic field. Further, we compare our results with the ones derived from time-dependent perturbation theory.

The paper proceeds as follows. In Sec. II, we describe the full Hamiltonian of an electron in both the atomic potential and a coherent photonic pulse. We give the full propagator and integrate over the photonic field. In Sec. III, we present a path-integral formalism for the dynamics of the electron. In Sec. IV, in order to avoid any additional complications, we apply the present theory to the ionization of hydrogen from its ground state due to the applied pulse. Certainly, the present method is applicable to either the ionization or to any bound-bound transition of any atom or molecule. Finally, in Sec. V we give our conclusions.

II. SYSTEM HAMILTONIAN AND PATH INTEGRATION

The system Hamiltonian H can be written as a sum of three terms: The electron Hamiltonian H_e in the atomic field, the photonic field part H_f, and the interaction term H_I,

$$H = H_e + H_f + H_I. \tag{1}$$

In particular, the electron Hamiltonian is given as

$$H_e = \frac{1}{2}\vec{p}^2 + V(\vec{r}), \tag{2}$$

where $V(\vec{r})$ is the atomic potential.

The Hamiltonian of the one-mode coherent light has the form

$$H_f = \omega a^\dagger a. \tag{3}$$

Finally, the interaction Hamiltonian in the Power-Zienau-Woolley formalism is given as

$$H_I = -e\vec{r}\cdot\vec{E}_f(\vec{r},t). \tag{4}$$

The field operator of the photonic field in a large volume V is given as

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$$\vec{E}_f(\vec{r},t) = \frac{1}{\sqrt{V}} il(\omega)\wp(t)\hat{\varepsilon}[ae^{i\vec{k}\cdot\vec{r}} - a^\dagger e^{-i\vec{k}\cdot\vec{r}}], \tag{5}$$

where $l(\omega)$ is a real function of frequency, given as $l(\omega) = \sqrt{\hbar\omega/2\varepsilon_0}$, $\hat{\varepsilon}$ is the polarization along the z axis, $\wp(t)$ is a time-dependent function modeling the pulse shape, and ε_0 is the vacuum dielectric constant. Then in the dipole (long-wavelength) approximation [$e^{i\vec{k}\cdot\vec{r}} \approx 1$ in Eq. (5)], H_I takes the form

$$H_I = g(t)(a - a^\dagger), \tag{6}$$

where

$$g(t) = -\frac{1}{\sqrt{V}} iel(\omega)\wp(t)\hat{\varepsilon}\cdot\vec{r}(t). \tag{7}$$

Let us combine the photonic field variables in the term

$$H_0(a^\dagger, a; t) = H_f + H_I = \omega a^\dagger a + g(t)a + g^*(t)a^\dagger. \tag{8}$$

The propagator between the initial and final states corresponding to the Hamiltonian (1) can be obtained by integrating over both the space and photonic field variables. At first we integrate over the photonic field variables, which appear only in H_0 [Eq. (8)]. Then there results the following path integral of only the spatial variables [17]:

$$K(\alpha_f,\vec{r}_f;\alpha_i,\vec{r}_i;t) = \int D\vec{r}(\tau)\frac{D\vec{p}(\tau)}{(2\pi)^3}\exp\left(i\int_0^t d\tau\left[\vec{p}(\tau)\cdot\dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau))\right] - i\int_0^t d\tau g(\tau)Z(\tau) - \frac{1}{2}(|\alpha_f|^2 + |\alpha_i|^2) + Y(t)\alpha_f^*\alpha_i + Z(t)\alpha_f^* - i\alpha_i X(t)\right), \tag{9}$$

where $Y(t)$, $X(t)$, and $Z(t)$ are given as (cf. [17])

$$Y(t) = \exp\left[-i\int_0^t d\tau\omega(\tau)\right] = \exp(-i\omega t), \tag{10}$$

$$X(t) = \int_0^t d\tau g(\tau)Y(\tau), \tag{11}$$

$$Z(t) = -i\int_0^t d\tau g^*(\tau)\exp\left[-i\int_\tau^t d\tau'\omega(\tau')\right]. \tag{12}$$

The propagator (9) with diagonal field variables ($\alpha_i = \alpha_f = \alpha$) can be written as

$$K(\alpha,\vec{r}_f;\alpha,\vec{r}_i;t) = \int D\vec{r}(\tau)\frac{D\vec{p}(\tau)}{(2\pi)^3}\exp\left(i\int_0^t d\tau\left[\vec{p}(\tau)\cdot\dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau))\right] + A - B|\alpha|^2 + D_1\alpha + D\alpha^*\right), \tag{13}$$

where the parameters are given as

$$A(t) = -\frac{1}{V}e^2 l^2(\omega)\int_0^t d\tau\int_0^\tau d\rho\wp(\tau)\hat{\varepsilon}\cdot\vec{r}(\tau) \times\wp(\rho)\hat{\varepsilon}\cdot\vec{r}(\rho)e^{i\omega(\rho-\tau)}, \tag{14}$$

$$B(t) = 1 - Y(t) = 1 - e^{-i\omega t}, \tag{15}$$

$$D(t) = \frac{1}{\sqrt{V}}el(\omega)\int_0^t d\tau\wp(\tau)\hat{\varepsilon}\cdot\vec{r}(\tau)e^{i\omega\tau}e^{-i\omega t}, \tag{16}$$

$$D_1(t) = -\frac{1}{\sqrt{V}}el(\omega)\int_0^t d\tau\wp(\tau)\hat{\varepsilon}\cdot\vec{r}(\tau)e^{-i\omega\tau}. \tag{17}$$

We consider that we have a field transition between two coherent states $|\beta\rangle$ and $|\gamma\rangle$. We should notice that photonic transitions between other kinds of states, such as excited coherent states, etc., could be treated similarly.

Now we can integrate the propagator (13) over the field variable α between the final $|\gamma\rangle$ and the initial $|\beta\rangle$ coherent field states by using their standard projections, e.g.,

$$\langle\alpha|\gamma\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\gamma|^2 + \alpha^*\gamma\right) \tag{18}$$

for the $|\gamma\rangle$ state, and similarly for the $|\beta\rangle$ state and integrating with the coherent-state representation measure, to obtain the following reduced propagator for the motion of the electron:

$$\tilde{K}^{\gamma,\beta}(\vec{r}_f,\vec{r}_i,t) = C(t)\int D\vec{r}(\tau)\frac{D\vec{p}(\tau)}{(2\pi)^3}\exp\{iS_{\text{tot}}[\vec{p},\vec{r},\tau]\} \equiv C(t)\tilde{K}_0(\vec{r}_f,\vec{r}_i,t), \tag{19}$$

where

$$C(t) = \frac{\exp\left(\frac{\beta\gamma^*}{B(t)} - \frac{1}{2}|\beta|^2 - \frac{1}{2}|\gamma|^2\right)}{B(t)}, \tag{20a}$$

the action is

$$S_{\rm tot}[\vec{p},\vec{r},\tau]=\int_0^t\left(\vec{p}(\tau)\cdot\dot{\vec{r}}(\tau)-\frac{\vec{p}^2(\tau)}{2}-V(\vec{r}(\tau))\right.$$
$$\left.+\frac{1}{\sqrt{V}}el(\omega)\wp(\tau)[u(t,\tau)\gamma^*-u^*(t,\tau)\beta]\hat{\varepsilon}\cdot\vec{r}(\tau)\right)d\tau$$
$$+\frac{1}{V}e^2l^2(\omega)\int_0^t d\tau\int_0^\tau d\rho\wp(\tau)\hat{\varepsilon}\cdot\vec{r}(\tau)\wp(\rho)\hat{\varepsilon}\cdot\vec{r}(\rho)$$
$$\times\xi(t,\tau-\rho) \tag{20b}$$

and the functions $u(t,\tau)$, $\xi(t,\tau-\rho)$ (cf. [17]) are given as

$$u(t,\tau)=-i\frac{e^{i\omega\tau}}{e^{i\omega t}-1}, \tag{21a}$$

$$\xi(t,\tau-\rho)=ie^{-i\omega(\tau-\rho)}+i\frac{2}{e^{i\omega t}-1}\cos[\omega(\tau-\rho)]. \tag{21b}$$

We can use the following identity in order to calculate the contribution of the factor $C(t)$ in Eq. (19). For arbitrary $A(t)$, on using the identities

$$\frac{1}{B(t)}=\frac{1}{1-\exp(-i\omega t)}$$
$$=\frac{1}{2}-\frac{1}{2}i\cot\left(\frac{\omega t}{2}\right)=\frac{1}{2}-\frac{i}{\omega}\sum_{m=-\infty}^{\infty}\frac{1}{t-\frac{2\pi m}{\omega}}, \tag{22a}$$

we can obtain the following formula after a direct Fourier transform:

$$\int_{-\infty}^{\infty}\frac{A(t)}{B(t)}e^{ift}dt=\frac{1}{2}\int_{-\infty}^{\infty}A(t)e^{ift}dt+\frac{\pi}{\omega}\sum_{m=-\infty}^{\infty}A\left(\frac{2\pi m}{\omega}\right)$$
$$\times\exp\left(if\frac{2\pi m}{\omega}\right). \tag{22b}$$

Finally, on using an inverse Fourier transform we obtain the following functional identity:

$$\frac{A(t)}{B(t)}=A(t)\left[\frac{1}{2}+\frac{\pi}{\omega}\sum_{m=-\infty}^{\infty}\delta\left(\frac{2m\pi}{\omega}-t\right)\right]$$
$$=A(t)\left[\frac{1}{2}+\frac{1}{2}\sum_{m=-\infty}^{\infty}\delta\left(m-\frac{\omega t}{2\pi}\right)\right]. \tag{22c}$$

In the above expressions, the summation is to be performed symmetrically. The δ functions do not contribute in the final expressions as at the specific times introduced by them the term on the exponent in the Monte Carlo expression (see Sec. III) becomes $-\infty$. Moreover, the measure of all those times is zero.

Now due to the large volume V, we shall approximate the exact action (20b) by neglecting in the Taylor expansion

$$\hat{\varepsilon}\cdot\vec{r}(\rho)=\hat{\varepsilon}\cdot\vec{r}(\tau)-(\rho-\tau)\hat{\varepsilon}\cdot\dot{\vec{r}}(\tau)+\cdots \tag{23}$$

higher terms than the first, as they are going to involve powers of higher order in V in the denominator.

To demonstrate this, we consider the action (20b) and we derive the equation of motion of the electron by using Lagrange's equation and the Lagrangian in Eq. (20b) in the absence of $V(\vec{r})$. So the part of the Lagrangian that interests us is

$$L=\frac{\dot{\vec{r}}^2(\tau)}{2}+\frac{1}{\sqrt{V}}el(\omega)\wp(\tau)[u(t,\tau)\gamma^*-u^*(t,\tau)\beta]\hat{\varepsilon}\cdot\vec{r}(\tau)$$
$$+\frac{1}{V}e^2l^2(\omega)\wp(\tau)\hat{\varepsilon}\cdot\vec{r}(\tau)\int_0^\tau d\rho\wp(\rho)\hat{\varepsilon}\cdot\vec{r}(\rho)\xi(t,\tau-\rho) \tag{24}$$

and the equation of motion reads

$$\ddot{\vec{r}}(\tau)=2\frac{1}{V}e^2l^2(\omega)\wp(\tau)\hat{\varepsilon}\int_0^\tau d\rho\wp(\rho)\hat{\varepsilon}\cdot\vec{r}(\rho)\xi(t,\tau-\rho)$$
$$+\hat{\varepsilon}\frac{1}{\sqrt{V}}el(\omega)\wp(\tau)[u(t,\tau)\gamma^*-u^*(t,\tau)\beta]. \tag{25}$$

Therefore, $\dot{\vec{r}}(\tau)$ is negligible compared with $\vec{r}(\tau)$ as $V\to\infty$.

In the case of the presence of $V(\vec{r})$, we perform a full-order perturbation expansion of the full propagator (19) with respect to the potential term

$$\tilde{K}_0=T+TVT+TVTVT+\cdots. \tag{26}$$

Then the propagator T in the expansion will be the one of the electron in the photonic field [17], for which the approximation (23) as discussed above is valid. Then, we sum back to obtain the final full propagator, thus maintaining the same approximation for the total propagator as well. This is also intuitively reasonable, because if the change in the position $\vec{r}$, due to the photonic interaction, is small when the electron is free, it is even smaller when it is bound. Notice that the expansion (26) may converge very slowly, but since it is a full-order expansion it does not matter.

Following this and by setting

$$\nu(t,\tau)=\wp(\tau)\int_0^\tau\wp(\rho)\xi(t,\tau-\rho)d\rho, \tag{27}$$

the action (20b) of the atomic electron in the presence of the photonic field becomes

$$S_{\rm tot}[\vec{p},\vec{r},\tau]=\int_0^t d\tau\left(\vec{p}(\tau)\cdot\dot{\vec{r}}(\tau)-\frac{\vec{p}^2(\tau)}{2}-V(\vec{r}(\tau))\right.$$
$$\left.+\frac{1}{\sqrt{V}}el(\omega)\wp(\tau)[u(t,\tau)\gamma^*-u^*(t,\tau)\beta]\hat{\varepsilon}\cdot\vec{r}(\tau)\right)$$
$$+\frac{1}{V}e^2l^2(\omega)\int_0^t d\tau[\hat{\varepsilon}\cdot\vec{r}(\tau)]^2\nu(t,\tau). \tag{28a}$$

This action corresponds to the effective Hamiltonian

$$H_{\rm eff} = H_e - \frac{1}{\sqrt{V}} el(\omega)\wp(\tau)[u(t,\tau)\gamma^* - u^*(t,\tau)\beta]\hat{\varepsilon}\cdot\vec{r}(\tau)$$

$$- \frac{1}{V} e^2 l^2(\omega)[\hat{\varepsilon}\cdot\vec{r}(\tau)]^2 \nu(t,\tau), \tag{28b}$$

where H_e in the case of the present problem is defined in (2). The term of order $1/\sqrt{V}$ is due to the action of the photonic field on the active electron of the atom, while the term of order $1/V$ is due to the electromagnetic vacuum fluctuations. The latter term, although of higher order, is necessary to have a consistent path-integral calculation in the present formalism.

III. MONTE CARLO METHOD

Now we proceed to obtain a Monte Carlo expression for the above path integral. In its discrete form, the path integral $\tilde{K}_0(\vec{r}_f,\vec{r}_i.t)$ in Eq. (19) can be written as

$$\tilde{K}_0(\vec{r}_f,\vec{r}_i;t) = \lim_{N\to\infty}\prod_{n=1}^{N}\int_{-\infty}^{\infty} d\vec{r}_n \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{d\vec{p}_n}{(2\pi)^3}\right]\exp\left\{i\sum_{n=1}^{N+1} S_n\right\}, \tag{29a}$$

where $\varepsilon = t/(N+1)$.

In spherical coordinates, $d\vec{r}_n$ can be written as $d\vec{r}_n = r_n^2 \sin\vartheta_n dr_n d\vartheta_n d\varphi_n$.

On supposing that we have directed the z axis along the direction of the linear polarization $\hat{\varepsilon}$, S_n can take the form

$$S_n = \left(\vec{p}_n\cdot(\vec{r}_n - \vec{r}_{n-1}) - \varepsilon\frac{\vec{p}_n^2}{2} - \varepsilon V(r_n)\right.$$

$$+ \varepsilon\frac{\sqrt{2\pi\omega}}{\sqrt{V}}\frac{\chi_n}{\sqrt{-\,\mathrm{sgn}(\nu_n)}}\sqrt{-\,\mathrm{sgn}(\nu_n)}r_n\cos\vartheta_n$$

$$\left. + \varepsilon\frac{2\pi\omega}{V}[-\,\mathrm{sgn}(\nu_n)]\nu_n[\sqrt{-\,\mathrm{sgn}(\nu_n)}r_n\cos\vartheta_n]^2\right) \tag{29b}$$

in atomic units, where χ_n is given as

$$\chi_n = \wp(\tau_n)[u_n(t,\tau_n)\gamma^* - u_n^*(t,\tau_n)\beta], \tag{29c}$$

ν_n is the discrete form of the variable defined in Eq. (27), and all the functions with index n are evaluated at time $\tau_n = n\varepsilon$. Additionally, we notice that we have set $\vec{r}_0 = \vec{r}_i$ and $\vec{r}_{N+1} = \vec{r}_f$.

In Eq. (29b), we use the sign term in order to ensure integrability of the arising Gaussian integral [see Eq. (32) below].

The exponential term in Eq. (29a) can be written as

$$e^{iS_n} = \int_{-\infty}^{\infty} dw_n \delta[w_n - \sqrt{-\,\mathrm{sgn}(\nu_n)}r_n\cos\vartheta_n]e^{iS_n^w}, \tag{30a}$$

where

$$S_n^w = \vec{p}_n\cdot(\vec{r}_n - \vec{r}_{n-1}) - \varepsilon\frac{\vec{p}_n^2}{2} - \varepsilon V(r_n) - \mathrm{sgn}(\nu_n)\nu_n w_n^2$$

$$+ \frac{\chi_n}{\sqrt{-\,\mathrm{sgn}(\nu_n)}} w_n. \tag{30b}$$

The δ function can be written as

$$\delta[w_n - \sqrt{-\,\mathrm{sgn}(\nu_n)}r_n\cos\vartheta_n]$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda_n e^{+i\lambda_n w_n} e^{-i\lambda_n\sqrt{-\mathrm{sgn}(\nu_n)}r_n\cos\vartheta_n}$$

$$= \frac{1}{2\pi}\sum_{l_n=0}^{\infty}(2l_n+1)i^{l_n}P_{l_n}(\cos\vartheta_n)$$

$$\times\int_{-\infty}^{\infty} d\lambda_n e^{+i\lambda_n w_n} j_{l_n}[-\sqrt{-\,\mathrm{sgn}(\nu_n)}\lambda_n r_n], \tag{31}$$

where P_l are Legendre polynomials and j_l are spherical Bessel functions.

In order to transfer the factor $\sqrt{2\pi\omega}/\sqrt{V}$ in Eq. (29b) in other terms of the propagator and obtain Eq. (30b), we perform the transformation $\lambda_n \to (\sqrt{2\pi\omega}/\sqrt{V})\lambda_n$. Consequently, by changing the order of integration between w_n and λ_n in Eqs. (30a), (30b), and (31) and using the identity

$$\int_{-\infty}^{\infty} dw_n e^{+i\lambda_n w_n}\exp\left[\varepsilon\left(-\,\mathrm{sgn}(\nu_n)\nu_n w_n^2 + \frac{\chi_n}{\sqrt{-\,\mathrm{sgn}(\nu_n)}}w_n\right)\right]$$

$$= \sqrt{\frac{\pi}{\varepsilon\,\mathrm{sgn}(\nu_n)\nu_n}}\exp\left(-i\sqrt{-\,\mathrm{sgn}(\nu_n)}\frac{\chi_n\lambda_n}{2\nu_n}\right)$$

$$\times\exp\left[-\frac{\lambda_n^2 + \varepsilon^2\mathrm{sgn}(\nu_n)\chi_n^2}{4\varepsilon\,\mathrm{sgn}(\nu_n)\nu_n}\right], \tag{32}$$

we conclude that the following l- and n-dependent function appears in our final expressions:

$$F_n^l(r_n) = \sqrt{\frac{\pi}{\varepsilon\,\mathrm{sgn}(\nu_n)\nu_n}}$$

$$\times\int_{-\infty}^{\infty}\frac{d\lambda_n}{2\pi}\left\{j_l\left(\frac{-\sqrt{2\pi\omega}}{\sqrt{V}}\sqrt{-\,\mathrm{sgn}(\nu_n)}\lambda_n r_n\right)\right.$$

$$\times\exp\left(-i\sqrt{-\,\mathrm{sgn}(\nu_n)}\frac{\chi_n\lambda_n}{2\nu_n}\right)$$

$$\left.\times\exp\left(-\frac{\lambda_n^2 + \varepsilon^2\,\mathrm{sgn}(\nu_n)\chi_n^2}{4\varepsilon\,\mathrm{sgn}(\nu_n)\nu_n}\right)\right\}. \tag{33}$$

Notice that for each l the definite integral in the above function can be evaluated analytically [19] in a closed form involving sines, cosines, exponentials, and error functions.

Finally, on performing the integration over $\vec{p}_n$, $n = 1,2,\ldots$, and certain standard manipulations [20], we obtain the following expression:

$$\tilde{K}_0(\vec{r}_f,\vec{r}_i;t)=\frac{1}{\sqrt{(2\pi i\varepsilon)^3}}\prod_{n=1}^{N}\left[\int_0^\infty \frac{dr_n d\cos\vartheta_n d\varphi_n}{\sqrt{(2\pi i\varepsilon)^3}}\right]\times\prod_{n=1}^{N+1}\left[\sum_{l_n'=0}^{\infty}\sum_{l_n=0}^{\infty}\sum_{m_n=-l_n}^{l_n}(2l_n'+1)i^{l_n'}F_n^{l_n'}(r_n)\times P_{l_n'}(\cos\vartheta_n)Y_{l_nm_n}(\vartheta_n,\varphi_n)Y^*_{l_nm_n}(\vartheta_{n-1},\varphi_{n-1})\times\exp\left\{i\left(\frac{(r_n-r_{n-1})^2}{2\varepsilon}-\varepsilon\frac{l_n(l_n+1)}{2r_nr_{n-1}}-\varepsilon V(r_n)\right)\right\}\right]. \tag{34}$$

On keeping leading terms in $V^{-1/2}$ (V is large), i.e., the first nonzero term with respect to l_n' in Eq. (34), we obtain, for a partition size of N slices, the following expression:

$$\tilde{K}_0(\vec{r}_f,\vec{r}_i;t)=\sum_{l=0}^{\infty}\sum_{q=0}^{\infty}\sum_{m=-q}^{q}\tilde{K}^{(N)}_{lqm}(r_f,r_i;t)(2l+1)i^lP_l(\cos\vartheta_f)\times Y_{qm}(\vartheta_f,\varphi_f)Y^*_{qm}(\vartheta_i,\varphi_i), \tag{35}$$

where

$$\tilde{K}^{(N)}_{lqm}(r_f,r_i;t)=F^l_{N+1}(r_f)\frac{1}{\sqrt{2\pi i\varepsilon}}\prod_{n=1}^{N}\left[\int_0^\infty\frac{dr_n}{\sqrt{2\pi i\varepsilon}}\right]\prod_{n=1}^{N}[F_n^0(r_n)]\times\exp\left\{i\sum_{n=1}^{N+1}\left(\frac{(r_n-r_{n-1})^2}{2\varepsilon}-\varepsilon\frac{q(q+1)}{2r_nr_{n-1}}-\varepsilon V(r_n)\right)\right\}. \tag{36}$$

Now we write expression (36) in the form

$$\tilde{K}^{(N)}_{lqm}(r_f,r_i;t)=F^l_{N+1}(r_f)\prod_{n=1}^{N}\left[\int_0^\infty dr_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n}{2\pi}\right]\times\prod_{n=1}^{N}[F_n^0(r_n)]\exp\left\{i\sum_{n=1}^{N+1}\left(p_n(r_n-r_{n-1})-\varepsilon\left[\frac{p_n^2}{2}+\frac{q(q+1)}{2r_nr_{n-1}}+V(r_n)\right]\right)\right\} \tag{37}$$

and apply the theory appearing in Ref. [21] to obtain a final standard expression to be used in the next section. It is

$$\tilde{K}^{(N)}_{lqm}(r_f,r_i;t)=\exp(-i\langle H_{1D}\rangle t)F^l_{N+1}(r_f)\prod_{n=1}^{N}[F_n^0(r_f)]\delta(r_f-r_i)+\frac{1}{\sqrt{N+1}}F^l_{N+1}(r_f)\prod_{n=1}^{N}\left[\int_0^\infty dr_n\right]\prod_{n=1}^{N}[F_n^0(r_n)]\times\left\{\prod_{n=1}^{N+1}[f(r_n,r_{n-1})]+i\prod_{n=1}^{N+1}[g(r_n,r_{n-1})]\right\}, \tag{38}$$

where

$$f(r_n,r_{n-1})=\frac{1}{2\pi\sqrt{2\pi\ \mathrm{Var}[V_c(r)]}t\ \sin\left(\langle H_{1D}\rangle t\right)}\times\exp\left\{-\frac{1}{2}\mathrm{Var}\left(\frac{p^2}{2}\right)t^2\sin^2(\langle H_{1D}\rangle t)\times(r_n-r_{n-1})^2-\frac{r_n^2}{2\ \mathrm{Var}[V_c(r)]t^2\sin^2\left(\langle H_{1D}\rangle\right)t}\right\}, \tag{39a}$$

$$g(r_n,r_{n-1})=\frac{1}{2\pi\sqrt{2\pi\ \mathrm{Var}[V_c(r)]}t\ \cos(\langle H_{1D}\rangle t)}\times\exp\left\{-\frac{1}{2}\mathrm{Var}\left(\frac{p^2}{2}\right)t^2\ \cos^2(\langle H_{1D}\rangle t)\times(r_n-r_{n-1})^2-\frac{r_n^2}{2\ \mathrm{Var}[V_c(r)]t^2\ \cos^2(\langle H_{1D}\rangle t)}\right\}, \tag{39b}$$

and the one-dimensional Hamiltonian H_{1D} is given as

$$H_{1D}=\frac{p^2}{2}+V_c(r), \tag{39c}$$

where

$$V_c(r)=\frac{q(q+1)}{2r^2}+V(r). \tag{39d}$$

The expectations are taken with respect to a standard sampling function relevant to the specific problem under consideration, as discussed in [21] as well.

We notice that in order to apply the above method, we have replaced the term r_{n-1} in the centrifugal term in Eq. (37) with the term r_n, a standard step discussed in [20] as well.

IV. APPLICATION TO HYDROGEN

Proceeding to an application of the present theory, we apply the above formalism to the case of the hydrogen atom. In that case, the potential is given as

$$V(\vec{r})=-\frac{1}{r}. \tag{40}$$

Additionally, the finite pulse duration is featured through a sine-square envelope. Then the $\wp(\tau)$ function of the above theory has the form

$$\wp(\tau)=\sin^2\left(\frac{\pi\tau}{\sigma}\right)\quad\text{when}\quad\tau\in[0,\sigma],$$

$$\wp(\tau)=0\quad\text{otherwise}, \tag{41}$$

where σ is the total duration of the pulse. Then, under the choice (41), Eq. (27) gives

$$\nu(t,\tau)=\sin^2\left(\frac{\pi\tau}{\sigma}\right)\frac{1}{2\omega^3\sigma^2-8\pi^2\omega}\left\{2\omega^2\sigma^2\sin^2\left(\frac{\pi\tau}{\sigma}\right)-8\pi^2\sin^2\left(\frac{\omega\tau}{2}\right)+2\pi\cot\left(\frac{\omega t}{2}\right)\times\left[\omega\sigma\sin\left(\frac{2\pi\tau}{\sigma}\right)-2\pi\sin(\omega\tau)\right]\right\}$$
$$\text{when}\quad \tau\in[0,\sigma], \tag{42}$$

$\nu(t,\tau)=0$ otherwise.

We proceed by calculating the probability density of the ionization from the ground state of hydrogen to its continuum. As in the present paper, we consider the case of a weak photonic field; we can suppose that the photonic field does not affect considerably those states. Then the final state of the electron with wave vector $\vec{k}=k(\sin\vartheta_k\cos\varphi_k,\sin\vartheta_k\sin\varphi_k,\cos\vartheta_k)$ is

$$\psi_f^{\vec{k}}(\vec{r},t)=\psi_f^{\vec{k}}(\vec{r})e^{-iw_pt}=\exp\left(\frac{\pi}{2k}\right)\Gamma\left(1+\frac{i}{k}\right)e^{i\vec{k}\cdot\vec{r}}{}_1F_1\times\left(-\frac{i}{k};1;-ikr-i\vec{k}\cdot\vec{r}\right)e^{-iw_pt} \tag{43a}$$

and it has energy

$$w_p=\frac{k^2}{2}. \tag{43b}$$

In our analytical manipulations, we use the expansion

$$\psi_f^{\vec{k}}(\vec{r})=\frac{4\pi}{k}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{\Gamma\left(1-\frac{i}{k}+l\right)}{\left|\Gamma\left(1-\frac{i}{k}+l\right)\right|}\times R_l^k(r)Y_{lm}^*(\vartheta,\varphi)Y_{lm}(\vartheta_k,\varphi_k), \tag{44a}$$

where

$$R_l^k(r)=\frac{\sqrt{8\pi k}}{\sqrt{1-\exp(-2\pi/k)}}\prod_{s=1}^{l}\left(\sqrt{s^2+\frac{1}{k^2}}\right)\frac{1}{(2l+1)!}\times(2kr)^le^{-ikr}{}_1F_1\left(\frac{i}{k}+l+1,2l+2,2ikr\right) \tag{44b}$$

and for $l=0$ the product in Eq. (44b) is replaced by unity.

Further, the initial state, i.e., hydrogen's ground state, is

$$\psi_i^{1s}(\vec{r},t)=\psi_i^{1s}(\vec{r})e^{-i\varepsilon_it}=R_{1s}(r)Y_{00}(\vartheta,\varphi)e^{-i\varepsilon_it}=2e^{-r}Y_{00}(\vartheta,\varphi)e^{-i\varepsilon_it}, \tag{45}$$

where $\varepsilon_i=-0.5$ is the energy of the $H(1s)$ state.

Then the transition amplitude from the initial state i at $t\to-\infty$ to the final continuum state f at $t\to+\infty$ may be evaluated at any time t; it is

$$A_{fi}=\langle\Phi_f^-(t)|\Phi_i^+(t)\rangle, \tag{46}$$

where $\Phi_f^-(\vec{r},t)$ and $\Phi_i^+(\vec{r},t)$ are exact solutions of the time-dependent Schrödinger equation, in which we use the effective Hamiltonian (28b) derived in Sec. II, subject to the asymptotic conditions

$$\Phi_f^-(\vec{r},t)\underset{t\to+\infty}{\to}\psi_f^{\vec{k}}(\vec{r},t), \tag{47a}$$

$$\Phi_i^+(\vec{r},t)\underset{t\to-\infty}{\to}\psi_i^{1s}(\vec{r},t). \tag{47b}$$

Then on adopting the prior form of the transition amplitude, that is

$$A_{fi}^-=\lim_{t\to-\infty}\langle\Phi_f^-(t)|\Phi_i^+(t)\rangle, \tag{48}$$

taking into account that the asymptotic initial and final states are orthogonal and performing some standard calculations, we finally obtain

$$A_{fi}^-=-\frac{1}{\sqrt{V}}el(\omega)\int_0^\sigma d\tau\wp(\tau)[u(\sigma,\tau)\gamma^*-u^*(\sigma,\tau)\beta]\times\langle\Phi_f^-(\tau)|\tilde{K}_0(\vec{r}_f,\vec{r}_i;\tau)(\hat{\varepsilon}\cdot\vec{r})|\psi_{1s}(\tau)\rangle$$
$$=-\frac{1}{\sqrt{V}}el(\omega)\int_0^\sigma d\tau\left\{\exp\left[i\left(\frac{k^2}{2}-\varepsilon_i\right)\tau\right]\wp(\tau)\times[u(\sigma,\tau)\gamma^*-u^*(\sigma,\tau)\beta]\times\int\int d\vec{r}_id\vec{r}_f\psi_f^{\vec{k}}(\vec{r}_f)\tilde{K}_0(\vec{r}_f,\vec{r}_i;\tau)(\hat{\varepsilon}\cdot\vec{r}_i)\psi_i^{1s}(\vec{r}_i)\right\}. \tag{49}$$

We notice that we have dropped the last higher-order term appearing in Eq. (28b). To evaluate Eq. (49), we apply the Monte Carlo method corresponding to formulas (38) and (39a)–(39d), and use as a sampling function for each term in Eq. (35), different from zero after the angular integration, the corresponding density $|R_l^k(r)|^2$ defined in Eq. (44b).

Finally, we conclude that the angular distribution of ejected electrons is given by

$$\frac{\partial^2P_{fi}^-}{\partial w_p\,\partial\Omega_k}=k|A_{fi}^-|^2, \tag{50}$$

where w_p and Ω_k are the energy and the direction corresponding to the impulse $\vec{k}$ of ejected electrons. Integrating over Ω_k we obtain the energy distribution $\partial P_{fi}^-/\partial w_p$, and one more integration over w_p gives the total probability to ionize an atom with one pulse.

We plot the distribution $\partial P_{fi}^-/\partial w_p$ versus the energy of an ejected electron for various pulse durations of the coherent photonic pulse in Fig. 1. In the calculations, we use $\omega=0.855$ a.u. [10,12] and $\sigma=100$ (photonic regime), $\sigma=40$ (lower limit of photonic regime), or $\sigma=8$ (collisional regime). We notice that, as expected in the collisional regime, there is not any apparent above-threshold ionization peak.

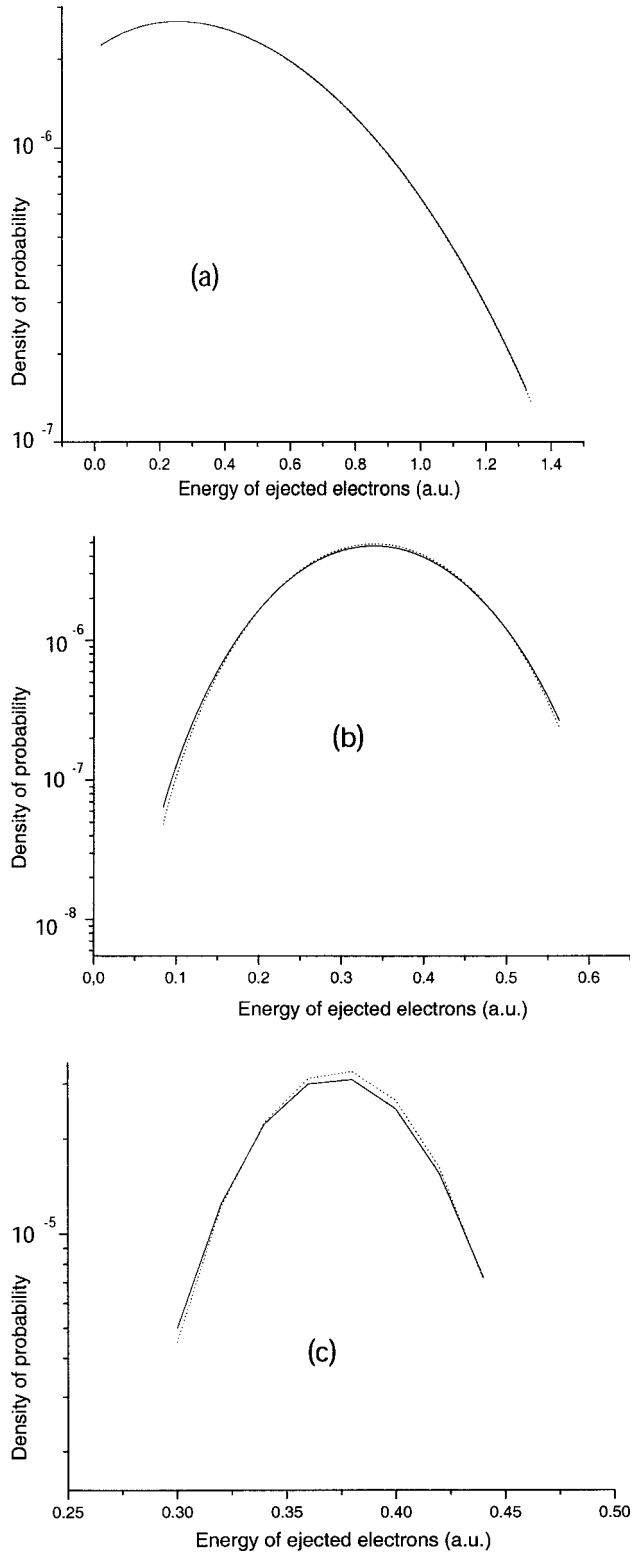

FIG. 1. Ionization of $H(1s)$: electron distribution (density probability per energy range) as a function of the energy of the ejected electron for a photon energy $\omega=0.855$, $\beta=1.0$ and various pulse lengths: (a) $\sigma=8$, (b) $\sigma=40$, and (c) $\sigma=100$. Solid line, present method. Dotted line, time-dependent perturbation theory. We have also set $V=10^8$. We notice that in the present range of the parameter's values the first term in Eq. (38) gives the major contribution and consequently the overall Monte Carlo error is very small.

Additionally, in the plots we compare the results of the present theory with the ones derived by time-dependent perturbation theory [22]. As the pulse duration increases, we have good agreement between the results from time-dependent perturbation theory and the present method only around the maximum of the one-photon above-threshold ionization peak. This is a consequence of the Monte Carlo integration error appearing in the present method, which prevents the exact reproduction of the oscillations appearing in other methods. See, for example, [12]. We notice that in all of our calculations we have used $N=8$, i.e., eight time slices. Further, the present method works only for small values of β due to machine accuracy. The range of β for which it is possible to apply the present method by programming in a 32 bit MATHMATICA environment is between zero and about three.

Moreover, the amplitude F_0 of the field of the pulse is related to the various other parameters in the present paper via the relation

$$F_0^2 = \omega \frac{|\beta|^2}{4\pi V}. \tag{51}$$

We notice that in the case of ionization by a coherent radiation pulse in cavity systems [14], the value of the β parameter seems more appropriate for the description of the pulse as the volume value is arbitrary and constant. Then the value of the β parameter is directly related with the mean number of photons present. Moreover, for ordinary volume values the amplitude of the field in Eq. (51) is definitely weak. So the present method appears as an alternative in the study of the interaction of pulses of a few photons with atoms or molecules, possibly in cavities [14]. Their exact intensity depends on the value of the volume of the experimental arrangement studied.

Finally, it is easy to observe that the one-photon above-threshold ionization peak in the plots corresponds to energy

$$E_1 = \varepsilon_i + \omega - U_p, \tag{52}$$

where ε_i is the ground-state energy of hydrogen and U_p is a ponderomotive energy. In perturbation conditions, one has

$$U_p = \frac{F_0^2}{4\omega^2}. \tag{53}$$

V. CONCLUSIONS

In the present paper, we modeled in a fully quantum-mechanical way the interaction of a coherent radiation pulse with an atom of one active electron. We extracted the propagator of the system, and specializing on the hydrogen we derived the ionization probability from the ground state to the continuum, for certain radiation parameters. We have restricted our calculations to small values of the β parameter implying weak fields for ordinary volumes, as on the one hand, in the case of strong fields a fully quantum-mechanical

treatment is not necessary and, on the other, the present method is not applicable for large values of β due to machine accuracy.

We notice that in the case of squeezed light what would have changed is only the specific form [15,16,23] of the functions $\nu(t,\tau)$ and $\chi(t,\tau)$ in the above theory.

The present model is simple and tractable and gives new aspects of the theory of photoionization. In the future, we intend to apply the present model when electric and magnetic fields are present as well.

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